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Li-ion battery capacity estimation: A geometrical approach

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HIGHLIGHTS

- A geometrical metric is proposed to estimate the battery capacity.
- Four geometrical features being sensitive to battery degradation are extracted.
- The law of battery degradation is recognized on an intrinsic manifold.
- Geodesic on the intrinsic manifold is used to estimate the battery capacity.
- A promising approach to battery assessment under different operating conditions.

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ABSTRACT

The majority of methods used for lithium-ion (Li-ion) capacity estimation are usually restricted to certain applications. Such methods often are time consuming and inconsistent with actual experimental data as well as depending on complicated battery operating and/or aging conditions. A geometrical approach to Li-ion battery capacity estimation is presented in this work. The proposed method utilizes four geometrical features that are sensitive to slight changes in the performance degradation of a Li-ion battery. The Laplacian Eigenmap method is used to establish an intrinsic manifold, and the geodesic on the manifold is used to estimate battery capacity. Tests are conducted based on data obtained under different operating and aging conditions provided by NASA Prognostics Center of Excellence. The evaluation results suggest that the proposed geometrical approach can be used to estimate Li-ion battery capacity accurately for the conditions given in this article.

1. Introduction

The high energy density of lithium and the lightweight of lithium batteries [1] have sparked interest in Li-ion batteries and resulted in a remarkably high number of studies aimed at improving the performance of such batteries [2]. The rate of capacity loss highly depends on operating conditions and permanent capacity loss over time; thus, accurate estimation of available battery capacity is often desired for reliability and better management of energy use [3].

Battery modeling and simulation [4–6] have undergone significant advancements over the past decade because of significant improvements in software capability and modern experimental techniques. Few attempts have been made to estimate Li-ion battery capacity. Zhang et al. [7] focused on characterizing the shifting electrical, chemical, and physical properties of anode, cathode, electrolyte, and current collectors. Fuller et al. [8] used a "first-principle" electrochemical model to estimate Li-polymer cell capacity. Spotnitz [9] incorporated solid electrolyte interphase (SEI) growth into Fuller's model and investigated the correlation of impedance change with capacity fade. In Ref. [4], an equivalent-circuit model was used to simulate cell performance, particularly the capacity fade phenomenon as influenced by thermal aging, which is one of the most influential factors affecting battery calendar life during storage, standby, or operational periods. An equation was proposed in Ref. [10], where two accurate state-of-charge (SOC) values are regarded as functions of the open circuit voltage (OCV), and the integrated current between these two values are sufficient to estimate the capacity of the battery cell. Chan et al.

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[11] applied an artificial neural network with single input and single output to build a correlation between discharge current and capacity for lead–acid batteries. They assumed that battery aging and degradation do not significantly affect capacity estimation. However, this assumption does not apply to Li-ion batteries. An extended Kalman filter [12] has also been used for capacity estimation based on the specific state/parameter models involved. In Ref. [13], a multivariate linear model was established to determine the relationship between capacity and a multitude of inputs, including internal DC resistance, OCV, and temperature.

So far, most of the abovementioned models have largely contributed to accurate capacity estimation. However, some issues should be dealt with before battery capacity estimation models can be fully applied to real-world applications:

(1) Dependence on accurate models representing the dynamic behavior of batteries, which have been proven difficult to establish [14], as in Refs. [4–6,12,13];
(2) Electrochemical parameters and properties of batteries are required, as in Refs. [4,7–9];
(3) Reliance on accurate SOC values, which are also part of a significant and difficult research field, as in Ref. [10];
(4) OCV values are needed, which always require considerable time of rest, as in Refs. [10,13];
(5) Being inappropriate for different operating conditions, as in Refs. [11–13].

Based on the aforementioned issues, a geometrical approach that can effectively reflect the intrinsic degradation or health state of Li-ion batteries is proposed. First, four geometrical features that are highly sensitive to slight changes in the degradation of Li-ion batteries are used to adjust to real applications. Second, the Laplacian Eigenmap (LE) method is applied to establish an intrinsic manifold where geodesic distances are calculated as the metric of the estimated capacity of a Li-ion battery. Meanwhile, the approach removes the need to study complex electrochemical mechanisms, to establish models, and to consume various times of rest for testing.

2. Related works

2.1. LE

In this paper, LE is applied not only for dimensionality reduction but also for the establishment of a low-dimensional manifold where Li-ion battery capacity will be estimated. A manifold, in mathematics, is a topological space where each point of an n-dimensional manifold has a neighborhood that is homeomorphic to the n-dimensional Euclidean space [15].

2.1.1. General description of LE

We assume that a d-dimensional manifold M^d (nominated as output space) embedded in an m-dimensional space $\alpha_N \in \mathbb{R}^m$ (nominated as input space, $d < m$) can be described by a function

$$f : C \subset M^d \rightarrow \mathbb{R}^m,$$

where C is a compact subset of M^d with open interior. A set of data points $\alpha 1, \ldots, \alpha N$, where $\alpha_i \in \mathbb{R}^m$, are sampled with noise from the intrinsic manifold M^d; the relationship can be represented as follows:

$$\alpha i = f(\beta i) + \xi i, \quad i = 1, \ldots, N, \tag{1}$$

where ξ_i denotes noise. LE can be recognized as: The original data set α_i's in the higher dimensional manifold $\mathbb{R}^m$ is mapped (nonlinearly) to the data point β_i's in the estimation of the unknown lower dimensional manifold M^d, with $d < m$ [16].

2.1.2. Theory of LE

Given a data set with N points, for arbitrary point $A \in M^d$ with k nearest neighborhoods, we construct a weighted graph $G = (V,E)$ with edges connecting nearby points to one another with the assumption that the graph is connected. We consider the problem of mapping the weighted graph G to a line, such that the connected points stay as close together as possible. Let

$$\boldsymbol{y} = (y_1, y_2, \cdots, y_N)^T \quad \boldsymbol{x} = (x_1, x_2, \cdots, x_N)^T, \tag{2}$$

where $x_i, y_i \in \mathbb{R}$ is a coordinate value of the ith point in $\mathbb{R}^m$ and M^d. A reasonable map is to choose y_i's $\in$ R to minimize $\sum_{ij} (y_i - y_j)^2 W_{ij}$ under the appropriate constraints. The objective function minimizing the coordinate is an attempt to keep the similarity of distances between x_i and x_j in the lower dimensional manifold, where y_i and y_j lie. As a result, for any $\boldsymbol{y}$, we have

$$\frac{1}{2}\sum_{i,j}\left(y_i - y_j\right)^2 W_{ij} = \boldsymbol{y}^T L \boldsymbol{y}, \tag{3}$$

where, as before, $L=D-W$, which is positive semidefinite. Notably, W_{ij} is symmetric, and $Dii = \sum_j Wij$. Thus, $\sum_{i,j}(y_i - y_j)^2 W_{ij}$ can be written as

$$\begin{aligned}\sum_{i,j}\left(y_i^2 + y_j^2 - 2y_i y_j\right) W_{ij} &= \sum y_i^2 Dii + \sum y_j^2 Djj - 2\sum y_i y_j W_{ij} \\ &= 2\boldsymbol{y}^T L \boldsymbol{y},\end{aligned} \tag{4}$$

Therefore, the minimization problem reduces to fining

$$\arg\min_{\boldsymbol{y}^T D \boldsymbol{y} = 1} \boldsymbol{y}^T L \boldsymbol{y}$$

The constraint $\boldsymbol{y}^T D \boldsymbol{y} = 1$ removes an arbitrary scaling factor in the embedding. Matrix D provides a natural measure on the graph vertice. A larger value of D_{ii} (corresponding to the ith vertex) makes the vertex more "important." From Eq. (3), L is shown as a positive semidefinite matrix, and the vector $\boldsymbol{y}$ that minimizes the objective function is given by the minimum eigenvalue solution to the generalized eigenvalue problem $L\boldsymbol{y} = \lambda D \boldsymbol{y}$ with an additional constraint of orthogonality

$$\arg\min_{\substack{\boldsymbol{y}^T D \boldsymbol{y} = 1 \\ \boldsymbol{y}^T D \boldsymbol{1} = 0}} \boldsymbol{y}^T L \boldsymbol{y}$$

More generally, the embedding is given by the $N \times d$ matrix $Y = [\boldsymbol{y}_1 \boldsymbol{y}_2 \ldots \boldsymbol{y}_d]$, where the ith row, denoted by Y_i^T, provides the embedding coordinates of the ith vertex. Similarly, we need to minimize

$$\sum_{i,j} \|Y_i - Y_j\|^2 W_{ij} = tr\left(Y^T L Y\right), \tag{5}$$

This condition reduces to finding [17]

$$Y_{\text{opt}} = \arg\min_{Y^T D Y = \boldsymbol{1}} tr\left(Y^T L Y\right), \tag{6}$$

2.2. Time-window for mapping updating

LE provides a mapping $g = f^{-1}$ for the fixed set of data from high-dimensional space to low-dimensional space. Therefore, the mapping from $\mathbb{R}^m$ can be conveniently extracted to M^d. Theoretically, one can receive a corresponding low-dimensional point through

the mapping when given an arbitrary point in the high-dimensional space. However, in practice, we need to achieve reasonable results from the $\mathbb{R}^m$ made of the features extracted from real-world applications. Thus, we often need to update the mapping provided by LE to adjust to the new incoming data. A general method is the so-called "time-window," which can be set as one incoming point or any other number of incoming points with regard to a real-world application. A new updated mapping is derived when the number of new incoming points reaches the fixed "time-window." However, for large data sets of high dimensionality, a trade-off exists between computation time consumption and the accuracy of estimation.

2.3. Geodesic on a manifold: a geometrical metric of battery capacity

In mathematics, particularly differential geometry, a geodesic is a generalization of the notion of a "straight line" to "curved spaces". If this connection is the Levi–Civita connection induced by a Riemannian metric, then the geodesics are (locally) the shortest path between points in the space [18]. In addition, the geodesic distance of two points is the shortest path between the two points, lying on a geodesic, in the space.

Fig. 1 shows a geodesic on a "Swiss roll" data set in two dimensions. (a) For two arbitrary points p and q on a nonlinear manifold, their intrinsic similarity measured can be reflected more accurately by geodesic distance than by the Euclidean space. (b) The straight line between p and q in the plane unfolded from the "Swiss roll".

The approximation of geodesic distances on curved surfaces is an important computational geometric problem that appears in numerous applications ranging from computer graphics, medical imaging, geophysics, to robot motion planning and navigation.

The approach used to calculate the approximation of geodesic distances in this paper is the method based on the graph theory proposed by Tenenbaum et al. and published in Science in 2000 [19].

Notably, the space mentioned in this paper is the Swiss roll surface rather than the R^3 Euclidean space.

3. Li-ion battery capacity estimation

This section demonstrates how the proposed battery capacity estimation method can be applied and validated.

3.1. Description of the NASA Li-ion experimental data

The data used to validate the above approach were collected from a custom-built battery setup (http://ti.arc.nasa.gov/tech/dash/pcoe/battery-prognostics/lab-setup/) at the NASA Ames Prognostics Center of Excellence. The experimental setup primarily consists of a set of Li-ion cells (which may reside either inside or outside an environmental chamber), chargers, loads, EIS equipment for battery health monitoring, a suite of sensors (voltage, current, and temperature), some custom switching circuitry, data acquisition system, and a computer for control and analysis [20].

The experiments are conducted through three different operational profiles (charge, discharge, and impedance) at ambient temperature (AT) conditions. Charging is performed in a constant charge current (CC) mode at 1.5 A until the battery voltage reaches 4.2 V and continues in a constant voltage (CV) mode until the charge current drops to 20 mA. The discharge runs are stopped at different end-of-discharges (EODs). The experiments are conducted until the capacity decreases to specified end-of-life (EOL) criteria. To validate the efficiency of the proposed approach, the typical data (#5, #7, #29, and #54) shown in Table 1 are selected. These data generally exhibit different ATs (°C), discharge currents (DCs; ampere), EOD criteria (voltage), and EOL criteria (ratio of faded capacity to initial capacity) for comparison. The accuracy and precision of the estimation shown below is a representative of the performance on the other batteries.

Table 1
Typical data obtained under different operating conditions for use in testing the efficiency of the proposed estimation method, with AT, CC, DC, EOD, and EOLC representing ambient temperature, charge current, discharge current, end-of-discharge, and end-of-life criteria, respectively.

Label no.	AT	CC	DC	EOD	EOLC (%)
5	24	1.5	2	2.7	30
7	24	1.5	2	2.2	30
29	43	1.5	4	2.0	12.61
54	4	1.5	2	2.2	30

3.2. Geometrical feature extraction

In most real-world applications, the slight changes caused by different operating and aging conditions will affect the geometrical characteristics contained in curves of charging and discharging processes. Features or parameters that reliably represent the actual performance or degradation of Li-ion batteries must first be determined to estimate Li-ion battery capacity accurately. Given the different operating and aging conditions, these features must be highly adaptive to all of these situations. With the elaboration on the analysis of raw Li-ion battery data sets, four typical geometrical features extracted from the raw current curve in the charging

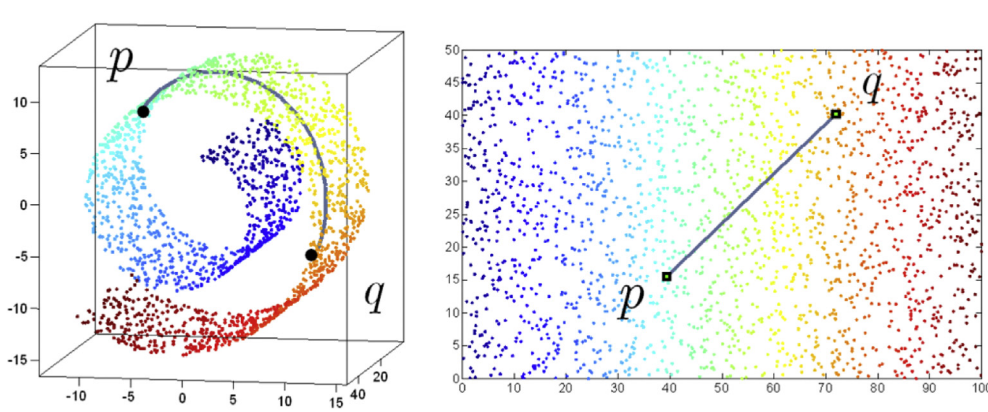

Fig. 1. Geodesic on a Swiss roll.

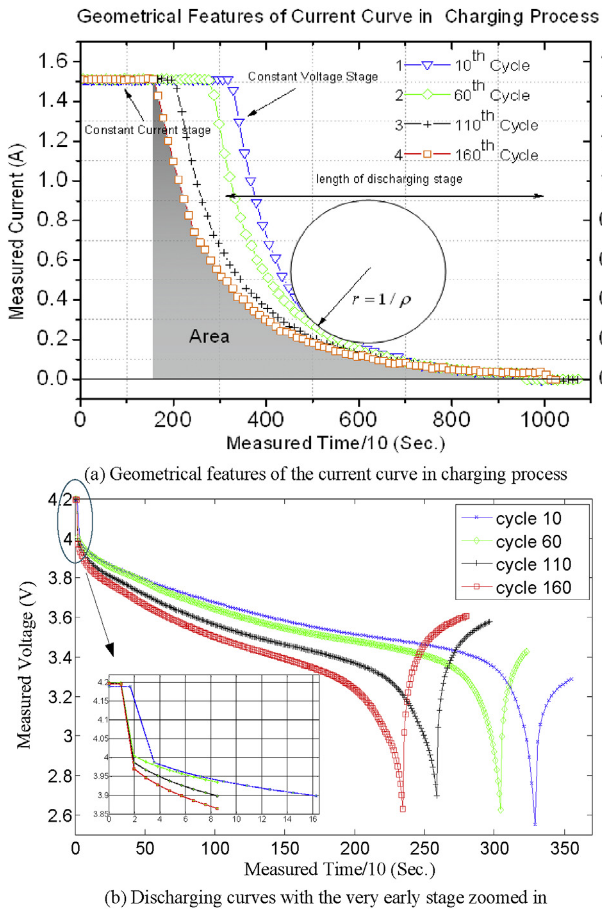

Fig. 2. Geometrical features extraction.

process and voltage curve in the discharging process are presented for use in Li-ion battery capacity estimation. All extracted geometrical features are sensitive to different operating and aging conditions. These features are described below.

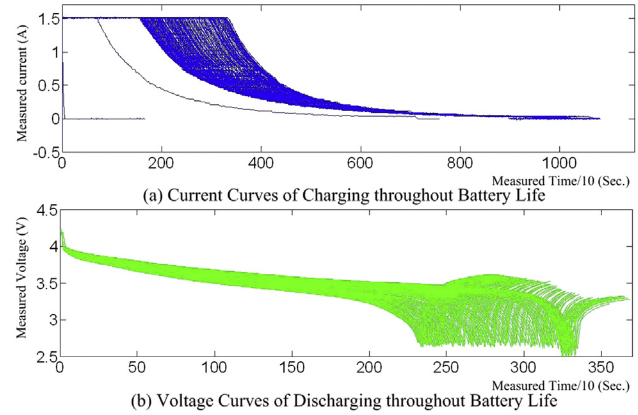

Fig. 4. Original charging/discharging curves of battery #5.

The current curves in the charging process (shown in Fig. 2a) and voltage curves in the discharging process (shown in Fig. 2b) of the 10th, 60th, 110th, and 160th cycles are depicted to illustrate the four extracted geometrical features. The charging process of a Li-ion battery can be divided into two stages, namely, the CC and CV stages. Three of the four geometrical features are extracted from the CV stages. Geometrical feature 1, *L*, is the length of CV stage of the current curve in the charging process; geometrical feature 2, *r*, represents the maximum radius of curvature in the curve of the CV stage; geometrical feature 3, *A*, denotes the area under the CV curve in the charging processes; and the fourth geometrical feature, *S*, indicates the maximum slope of a voltage curve during the early stage of the discharging process. Notably, the early stage is defined as the period during which the Li-ion voltage drops rapidly in this paper. In Fig. 2b, the early stages of the 10th, 60th, 110th, and 160th cycles have been zoomed in to obtain the detailed information.

All of the four geometrical features, *L*, *r*, *A*, and *S*, are shown in Fig. 2. The variances of these features over time are shown in Fig. 3. These features are good indicators for Li-ion battery performance degradation even under different operating and aging conditions.

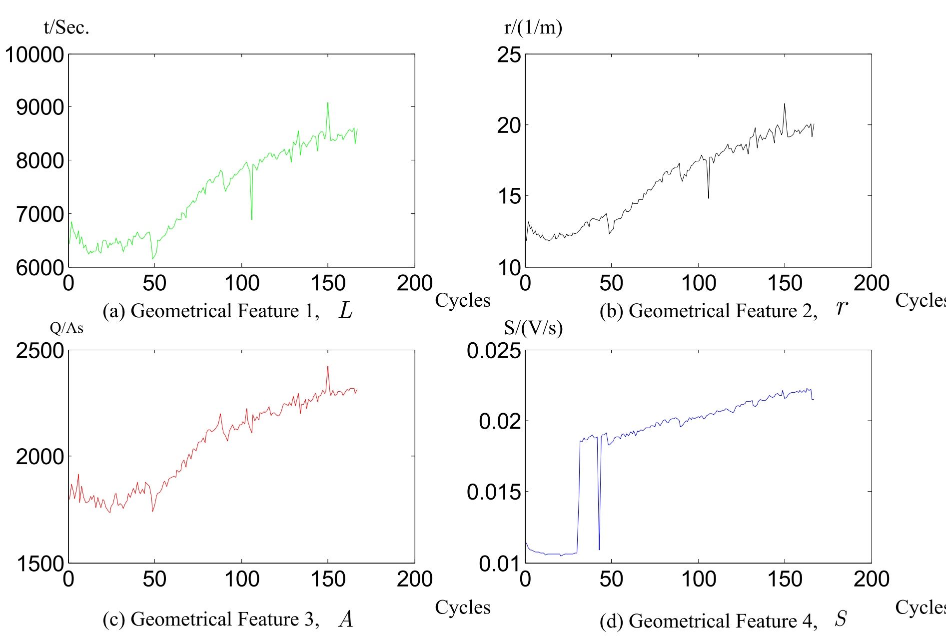

Fig. 3. Original geometric features extracted from the raw curves.

All these four geometrical features are used to estimate real battery capacity.

3.3. Manifold construction and geodesic distance computation for battery capacity estimation

3.3.1. Intrinsic manifold establishment

This section presents the establishment of an intrinsic manifold on which the law of battery performance degradation can be recognized and described well with the assumption that the intrinsic manifold has no relation with Li-ion battery operating conditions. The aforementioned LE method was originally used in manifold learning for dimensionality reduction and data representation. Through the LE method, representation can be constructed for data lying on a low-dimensional manifold embedded in a high-dimensional space. In the $\mathbb{R}^m$ space, $m = 4$ consists of the four geometrical features extracted from raw curves of Li-ion batteries. In the M^d space, where Li-ion battery capacity degradation can be well described, is the low-dimensional intrinsic manifold. The mapping $g = f^{-1}$ from $\mathbb{R}^m$ to M^d can be extracted based on the LE method. An analogous set of full-cycle of lifetime (ASL) raw experimental data was used as sample data to establish the mapping $g = f^{-1}$ for each of the four typical data sets. One point representing the Li-ion battery capacity in M^d can be obtained through the extracted mapping $g = f^{-1}$ when given a corresponding point in $\mathbb{R}^m$. For accurate capacity estimation, the "time-window" for mapping updating must be fixed. In this validation, the time-window is set to be one new incoming data point in the geometrical space $\mathbb{R}^m$.

3.3.2. Capacity estimation: geodesic distance computation on the established manifold

In this work, the geodesic on the intrinsic manifold M^d achieved by mapping $g = f^{-1}$ is used as a geometrical metric of battery health to estimate battery capacity. In addition, the geodesic distance between the first point and every other point on the intrinsic manifold is calculated using the graph theory. The estimated capacity of each point in $\mathbb{R}^m$ can be expressed as

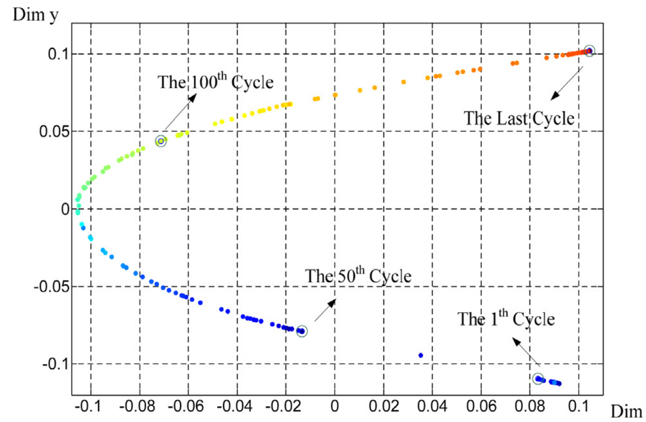

Fig. 6. Battery performance degradation on the intrinsic manifold established by the LE method.

$$\hat{C}_A = C_{A0} - \frac{geo_s}{geo_{EOL}}(C_{A0} - C_{EOL}), \tag{7}$$

where C_{A0} represents the initial capacity that is not always equal to the rated capacity, C_{EOL} is the capacity specified to the end charging/discharging cycle of validation data, geo_s denotes the geodesic distance between the first point and the point to estimate the capacity on the intrinsic manifold M^d, and geo_{EOL} indicates the geodesic between the first and last point on the intrinsic manifold of ASL.

4. Results and discussion

To illustrate the proposed technique, battery #5 is selected for demonstration. Fig. 4 shows the original current curves in the charging processes (Fig. 4a) and the voltage curves in the discharge

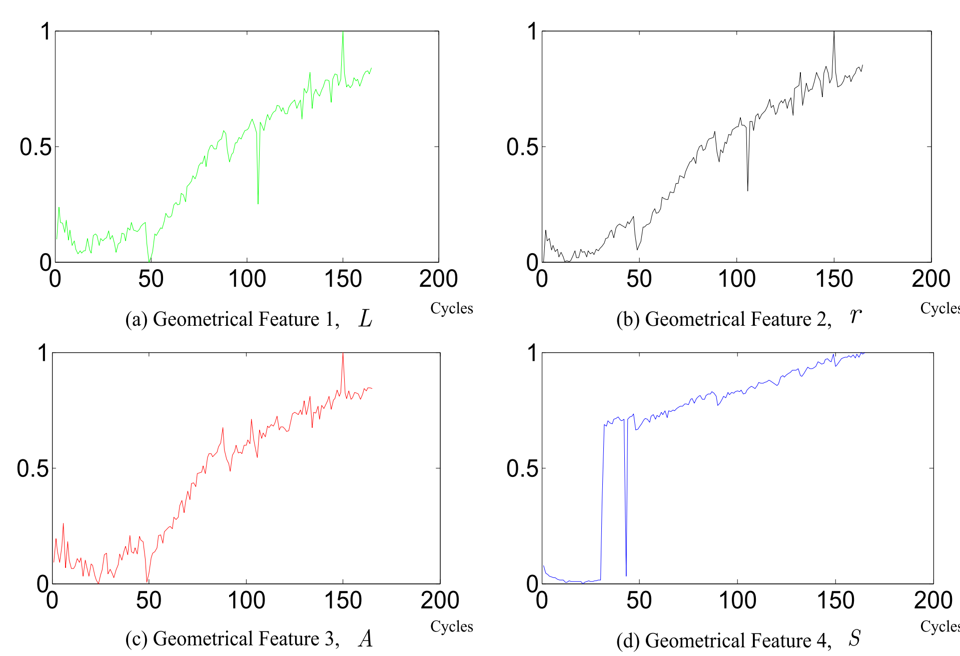

Fig. 5. Values and tendencies of the four extracted and normalized features.

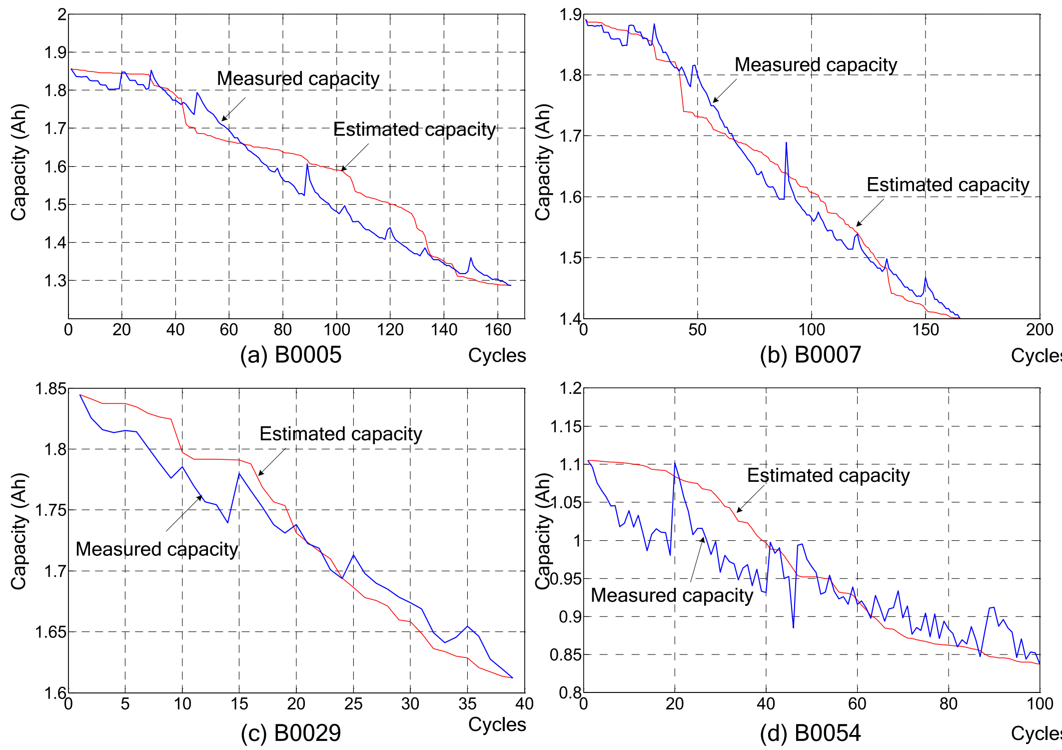

Fig. 7. Comparison between the measured and estimated capacities.

runs (Fig. 4b). Fig. 5 shows the four linear-normalized geometrical features extracted from the raw current and voltage curves.

Fig. 6 shows the intrinsic manifold based on the four normalized geometrical features established using the extracted mapping $g = f^{-1}$. The performance degradation at the 1st, 50th, 100th, and last cycle of battery charging/discharging in $\mathbb{R}^m$ is consistently scattered and clearly visible on the intrinsic manifold M^d. Notably, Fig. 6 shows the M^d of two-dimensional Dim x and Dim y satisfying the expression: $\sum \mathrm{Dim}x_i = 0$ and $\sum \mathrm{Dim}y_i = 0$.

The estimated capacity based on the geodesic distance computation on the intrinsic manifold using Eq. (7) and the measured capacity from all validation data (#5, #7, #29, and #54) were compared. Fig. 7 demonstrates the close tracking of the measured capacity under different operating and aging conditions. Table 2 shows that the estimated capacity maintains a high level of accuracy. The maximum and minimum of error 1 between estimated capacity and measured capacity are 4.48% and 1.85%, respectively. For error 2, the calculated values are 3.84% and 1.06%, respectively. Furthermore, the procedure and testing results show that the proposed method exhibits high accuracy in real-world applications.

Note: Error 1 = measured capacity C_A − estimated capacity $\hat{C}_A$

Error 2 = abs (measured capacity C_A − estimated capacity $\hat{C}_A$)/measured capacity C_A

Note: The cycling numbers of batteries used in this study are less than 200, so the accuracy of the approach for batteries with higher run-to-failure cycling numbers needs further validation.

Table 2
Estimation accuracy of available capacity based on the proposed method.

	#5	#7	#29	#54
Error 1 (%)	4.48	2.42	1.85	3.71
Error 2 (%)	2.93	1.49	1.06	3.84

5. Conclusions

A geometrical approach to Li-ion battery capacity estimation is presented. Slight changes in performance degradation can be derived using the proposed approach, which requires four geometrical features and uses the LE method and geodesic distance calculation. Validation is conducted based on the data obtained under different operating and aging conditions. The testing results demonstrate that the proposed geometrical approach can be used to estimate Li-ion battery capacity accurately under different operating and aging conditions. The procedure and testing results also show that the proposed method has high accuracy and can remove the need to study complex electrochemical mechanisms, to establish models, and to consume various times of rest for testing.

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References

[1] A. Barré, B. Deguilhemb, S. Grolleaub, M. Gérardb, F. Suarda, D. Riu, J. Power Sources 241 (2013) 680–689.
[2] M. Broussely, G. Archdale, J. Power Sources 136 (2004) 386–394.
[3] J.L. Zhang, J. Lee J, J. Power Sources 196 (2011) 6007–6014.
[4] B.Y. Liaw, R.G. Jungst, G. Nagasubramanian, H.L. Case, D.H. Doughty, J. Power Sources 140 (2005) 157–161.
[5] B. Wu, M. Mohammed, D. Brigham, R. Elder, R.E. White, J. Power Sources 101 (2001) 149–157.
[6] B.Y. Liaw, K.P. Bethune, X.G. Yang, J. Power Sources 110 (2) (2002) 330–340.
[7] X. Zhang, P.N. Ross Jr., R. Kostecki, F. Kong, S. Sloop, B. Kerr, K. Striebel, E.J. Cairns, F. McLarnon, J. Electrochem Soc. 148 (2001) A463–A470.
[8] T.F. Fuller, M. Doyle, J. Newman, J. Electrochem Soc. 141 (1994) 1–10.
[9] R. Spotnitz, J. Power Sources 113 (2003) 72–80.

[10] M. Einhorn, F.V. Conte, C. Kral, J. Fleig, in: 2010 IEEE International Conference on Sustainable Energy Technologies (ICSET), Kandy, Sri Lanka, 2010, pp. 1–6.
[11] C.C. Chan, E.W.C. Lo, W.X. Shen, J. Power Sources 87 (2000) 201–204.
[12] G.L. Plett, J. Power Sources 134 (2004) 277–292.
[13] S. Hoenig, H. Singh, T.G. Palanisamy, Method and Apparatus for Predicting the Available Energy of a Battery, 2001.
[14] X.D. Tang, X.F. Mao, J. Lin, B. Koch, 2011 American Control Conference on O'Farrell Street, San Francisco, CA, USA, June 29–July 01, 2011.
[15] http://en.wikipedia.org/wiki/Manifold.
[16] Z. Zhang, H. Zha, SIAM J. Sci. Comput. 26 (2005) 313–338.
[17] M. Belkin, P. Niyogi, Neural Comput. 15 (2003) 1373–1396.
[18] http://en.wikipedia.org/wiki/Geodesic.
[19] J.B. Tenenbaum, V.D. Silva, J.C. Langford, Science 290 (2000) 2319–2323.
[20] B. Saha, K. Goebel, Battery Data Set, NASA Ames Prognostics Data Repository, Moffett Field, CA, 2007. http://ti.arc.nasa.gov/tech/dash/pcoe/prognostic-data-repository/.